Overfitting and Remedies

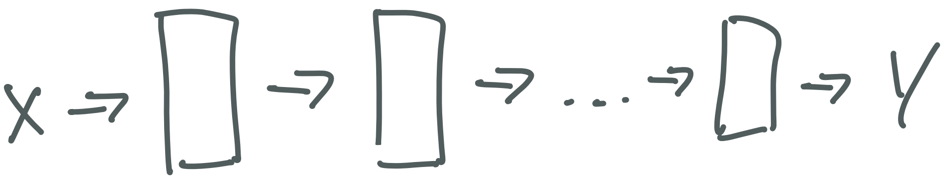
Find the perfect model complexity, Early stopping, Regularization, Dropout, Data augmentation, and Domain randomization

Outline

- Drawing recap for initialization and normalization
- Overfitting and its causes
- Overfitting remedies
  - Find the perfect model complexity
  - Early stopping
  - Regularization
  - Dropout
  - Data augmentation
  - Domain randomization

Recap: Parameter and Gradient Values

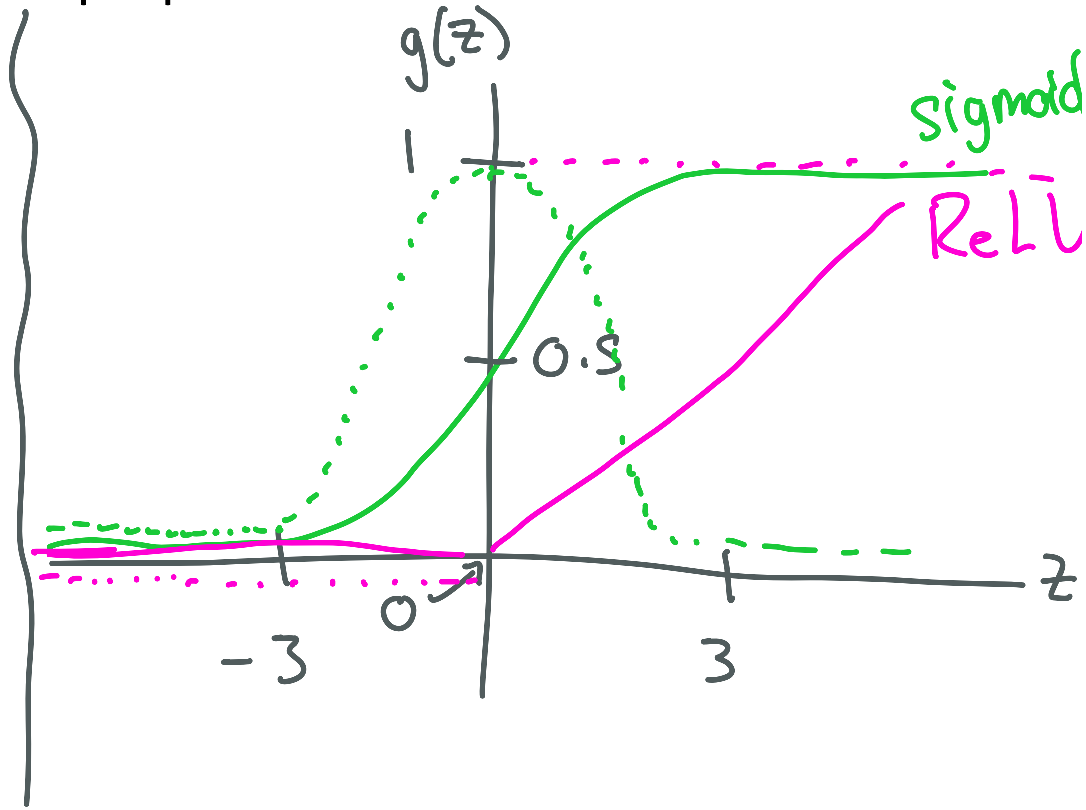
- Take five minutes to draw
- Example: activations with and without proper initialization and normalization



$$Z = A^{[l-1]} W^T + b$$

$$A^{[l]} = g(Z)$$

activation function



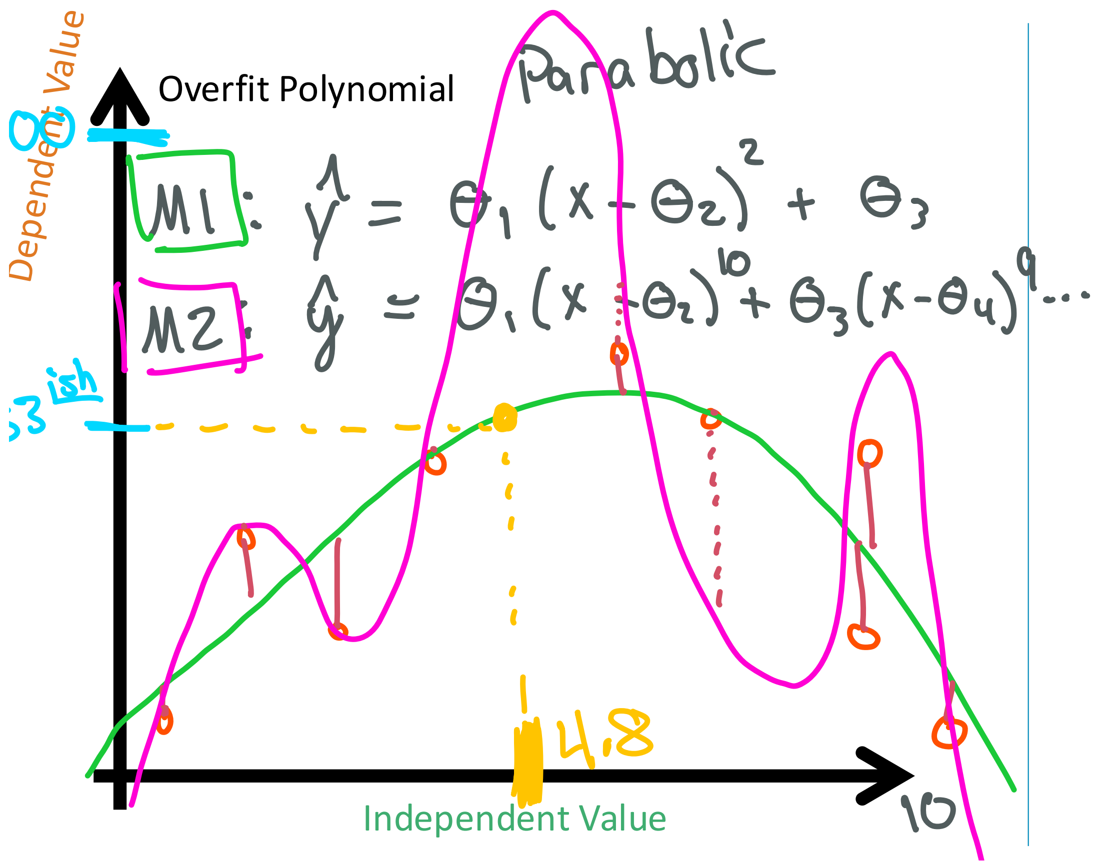
Classroom Etiquette

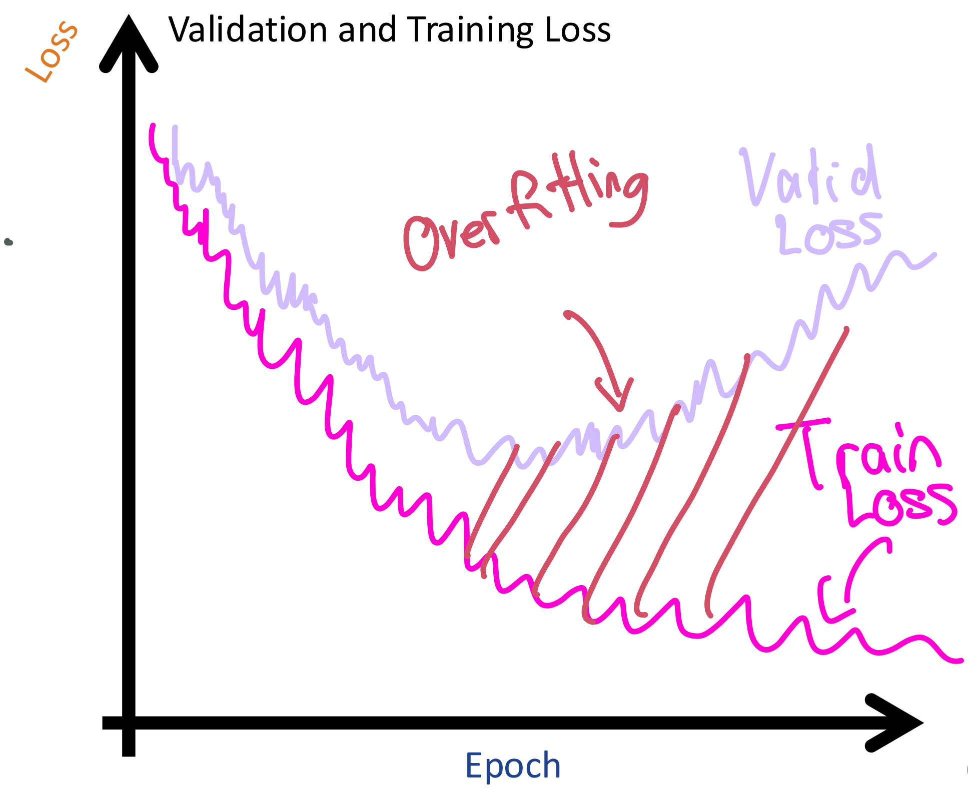
- We all want to look *effortlessly smart* in front of our peers.
  - It’s a fool’s errand. I’ve noticed it a bit in the class. Might be due to class makeup
- I’ve built my teaching philosophy around the “gift of failure”
  - You need to give me wrong answers
  - You need to be unafraid of being wrong
  - You need to be ready to fail

$\frac{1}{2}(\hat{y} - y)^2$ } $|\hat{y} - y|$

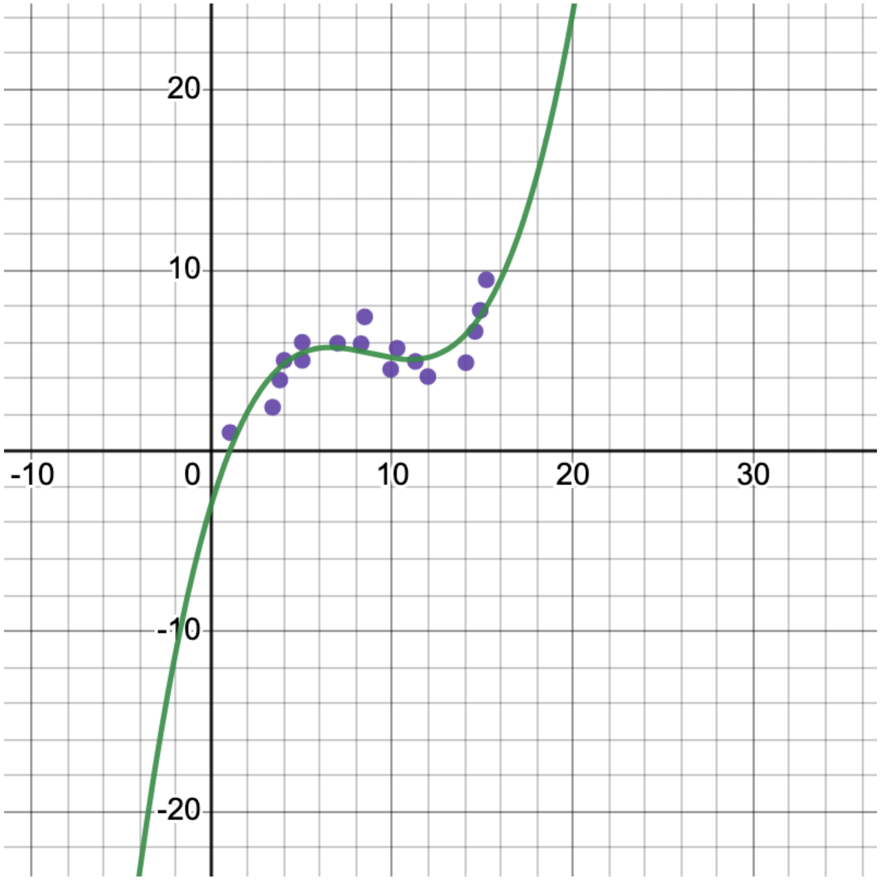
Overfitting

When your model learns/memorizes the training data and not some property that is useful for inference. *("I've seen this input before… the answer is X.")*





https://www.desmos.com/calculator/gysbxd1r0l



Causes of Overfitting

When your model learns/memorizes the training data and not some property that is useful for inference. *("I've seen this input before… the answer is X.")*

- The model is too complex
  - Too many parameters
  - Too deep
  - Too wide
  - Too much memory

Causes of Overfitting

When your model learns/memorizes the training data and not some property that is useful for inference. *("I've seen this input before… the answer is X.")*

50, 100

$$\hat{y} = \theta_1 x^{10} + \theta_2 x^{9} \cdots + \theta$$

- The model is too complex
  - Too many parameters
  - Too deep
  - Too wide
  - Too much memory
- Parameters are too large (large parameters lead to steep curves)
- The model was trained for too long
- The dataset was too small

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  - ✓ Find the perfect model complexity
  - ✓ Early stopping
  - Regularization
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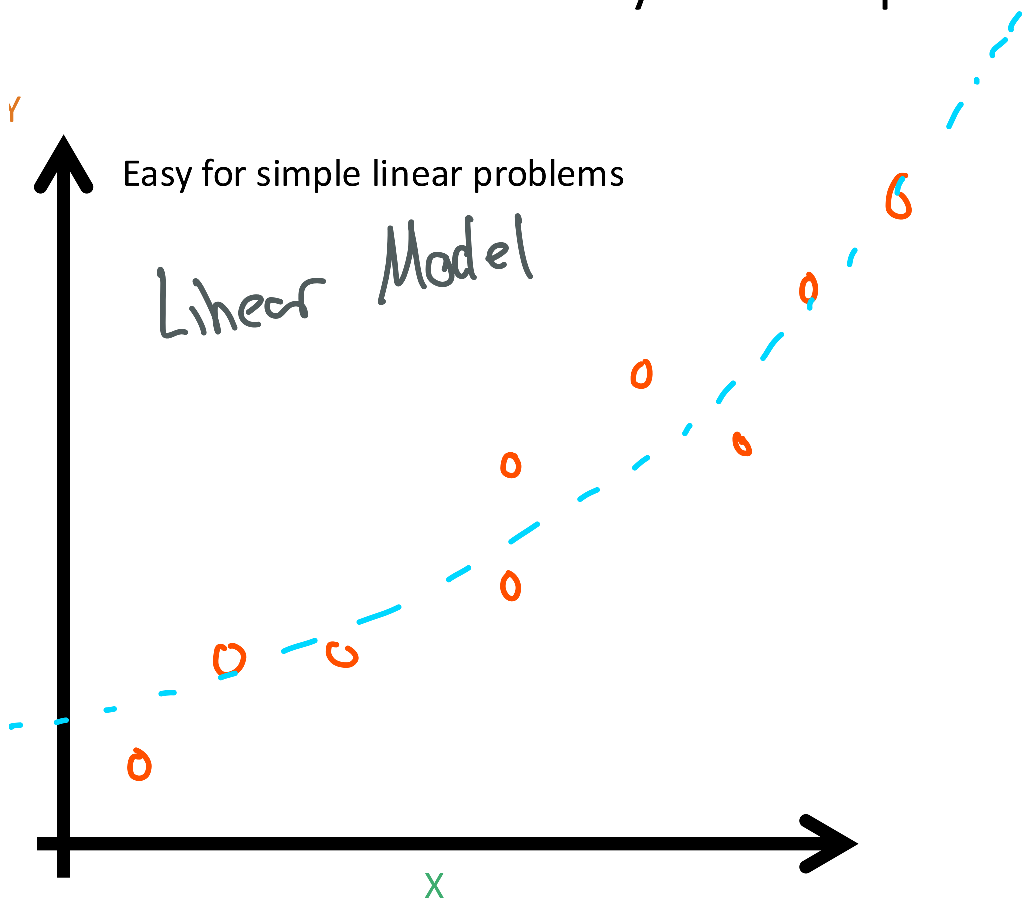
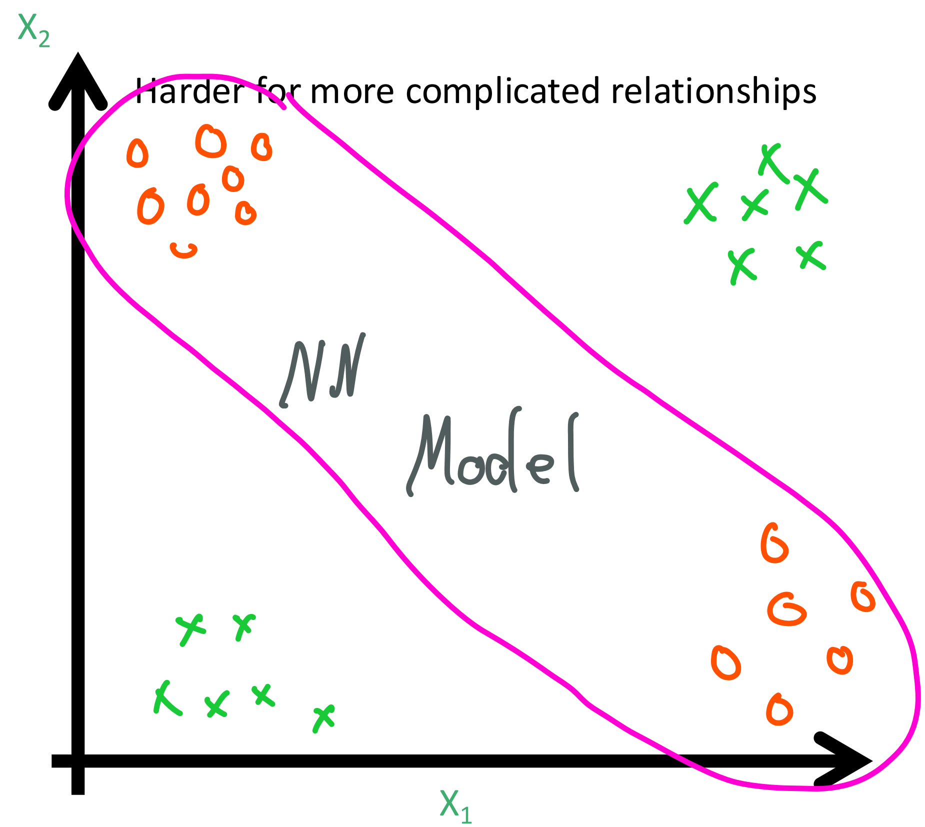
Remedy: Find the Perfect Model Complexity

We could theoretically find the perfect model complexity for each problem





Hyperparameter Search/Tuning

- Common methods for "finding" good hyperparameters include
  - Manual adjustments
  - Grid search
  - Random search
  - Bayesian optimization
  - Evolutionary optimization
  - (and others)

- I happen to prefer a simple "Twiddle Search"

```python
# Initial values
hyper_params = {
    "learning_rate": 0.1,
    "batch_size": 64,
    "num_layers": 10,
    "dropout": 0.5,
}

# Hyperparameter update factors
hyper_param_updates = {
    "learning_rate": {"up": lambda lr: lr * 10, "down": lambda lr: lr / 10},
    "batch_size": {"up": lambda bs: bs * 2, "down": lambda bs: max(bs // 2, 1)},
    "num_layers": {"up": lambda nl: nl * 2, "down": lambda nl: max(nl // 2, 1)},
    "dropout": {"up": lambda d: min(d + 0.1, 0.9), "down": lambda d: max(d - 0.1, 0.1)},
}

# Initial quality
best_metric_value = evaluate(hyper_params)

# Cache of hyperparameter value combinations
cache = {hyper_params.values(): best_metric_value}

attempts = 1
while not done(best_metric_value, attempts):

    # Choose a hyperparameter and an update direction
    hyper_param = choice(list(hyper_params.keys()))
    update_direction = choice(["up", "down"])

    # Update the hyperparameter
    current_value = hyper_params[hyper_param]
    new_value = hyper_param_updates[hyper_param][update_direction](current_value)
    new_hyper_params = {**hyper_params, hyper_param: new_value}

    # Check if the hyperparameter value combination has been evaluated before
    if new_hyper_params.values() in cache:
        continue

    attempts += 1

    # Evaluate the new hyperparameter value combination
    metric_value = evaluate(new_hyper_params)
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    if metric_value > best_metric_value:
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    print(f"Best metric value: {best_metric_value}: {hyper_params}")
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4

$4 \cdot 5 = 20$

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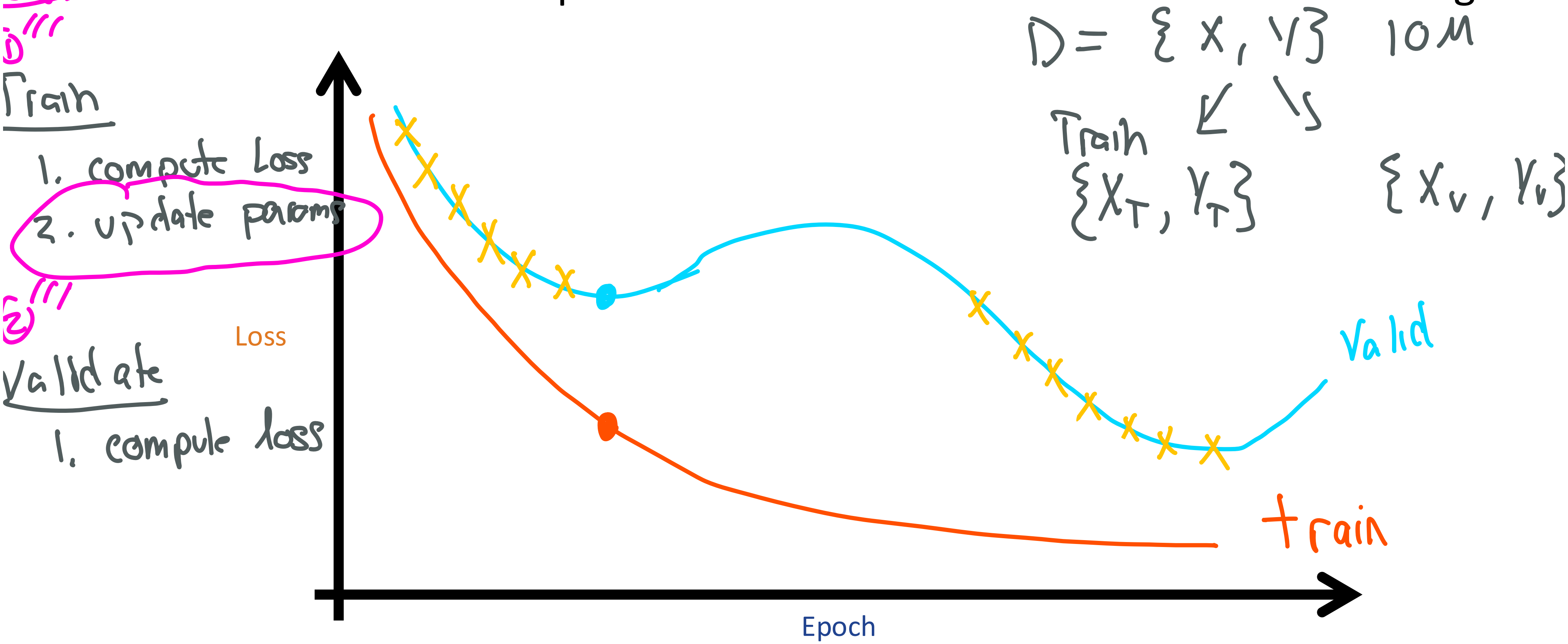
Remedy: Early Stopping and Checkpointing

- We can use the learned parameters from before we detected overfitting



Checkpointing

```
for epoch in range(num_epochs):
    model.train()
    for X, y in train_loader:
        yhat = model(X)
        loss = criterion(y, yhat)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

    model.eval()
    with torch.no_grad():
        for X, y in valid_loader:
            yhat = model(X)
            loss = criterion(y, yhat)
            metric = metrics(y, yhat, model, metric)

    if metric.is_best():
        model.save(f"model{epoch}.pkl")
```

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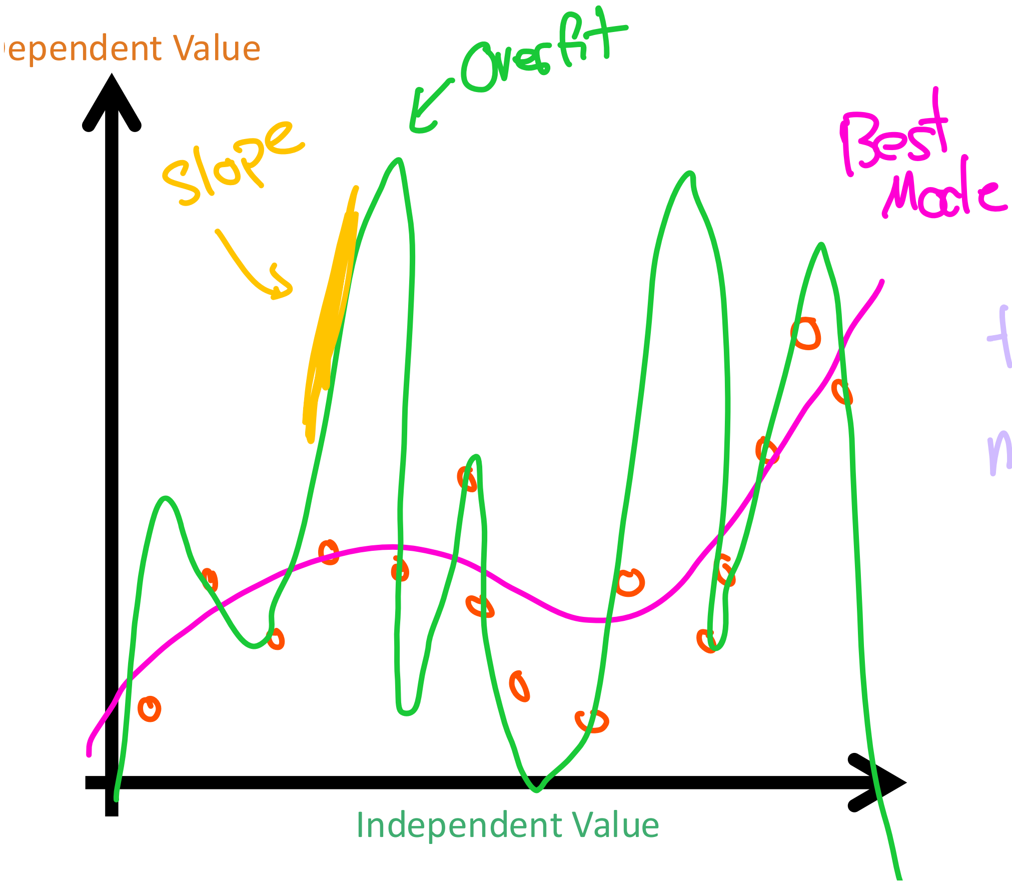
Remedy: Regularization

We can artificially *constrain* the parameter magnitudes <u>in our loss function</u>

(ie, optimize for lower parameter magnitudes)



$$\mathcal{L} = \frac{1}{2}(\hat{y} - y)^2$$

How would you change this function so that is also minimizes parameter values.

$$\mathcal{L} = \frac{1}{2}(\hat{y} - y)^2 + \lambda \frac{1}{2}\|\theta\|^2$$

weight decay

Derivative of ½ MSE with Regularization

$$\mathcal{L} = \frac{1}{2}(\hat{y} - y)^2 + \lambda \frac{1}{2}\|\theta\|^2$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = (\hat{y} - y)\hat{y}' + \lambda \theta$$

$$\theta_t := \theta_{t-1} - \alpha\left[(\hat{y} - y)\hat{y}' + \lambda \theta\right]$$

(1) θ is a large positive value
↳ reduce θ

(2) θ is a large negative value
↳ increase θ

} tend toward zero

$$\mathcal{L} = \frac{1}{2}(\hat{y} - y)^2 + \theta$$

$$\frac{\partial \mathcal{L}}{\partial \theta} = (\hat{y} - y)\hat{y}' + 1$$

$$\theta_t := \theta_{t-1} - \alpha((\hat{y} - y) + 1$$

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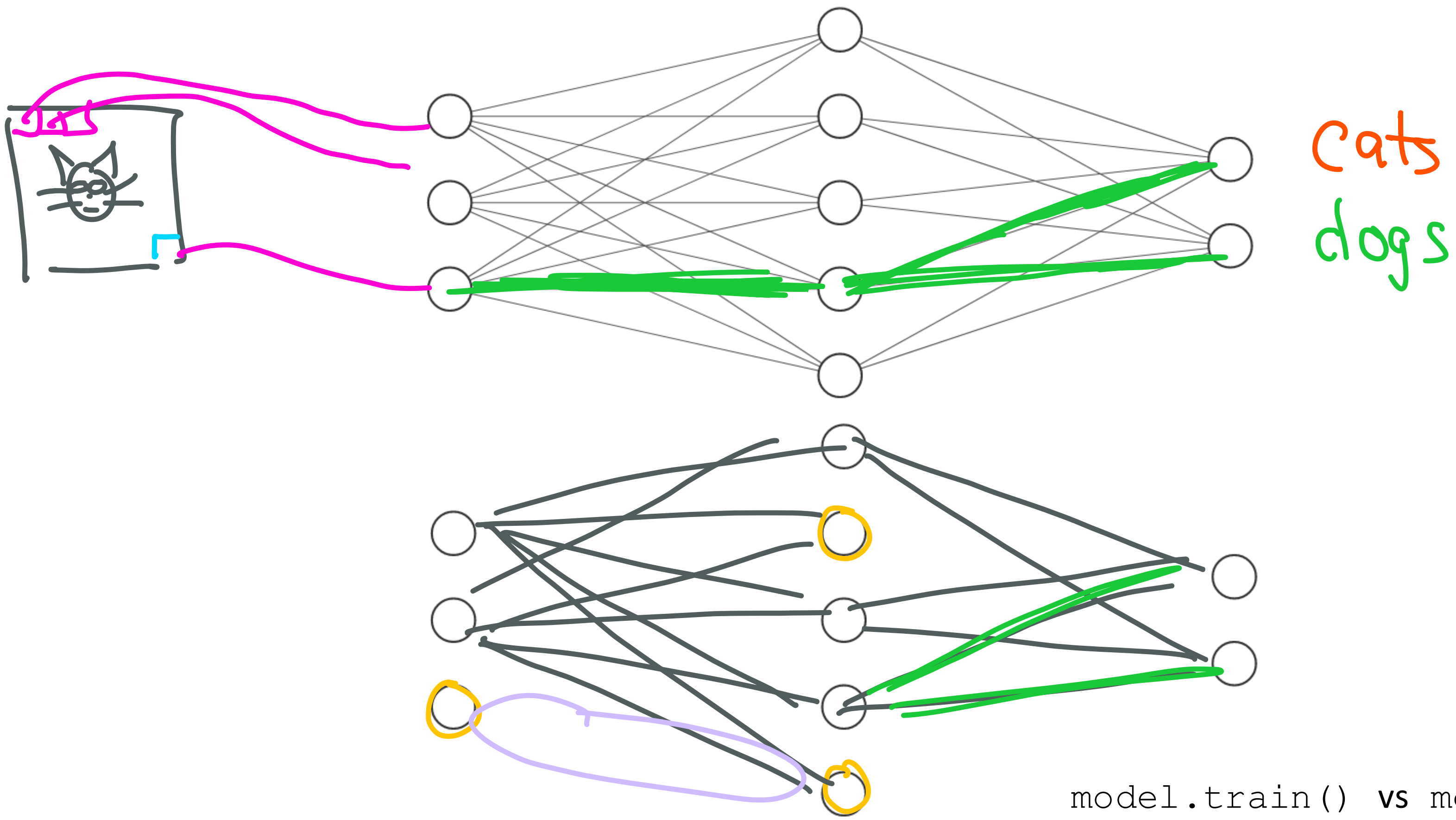
Remedy: Dropout

We can train the model in such a way that breaks memorization



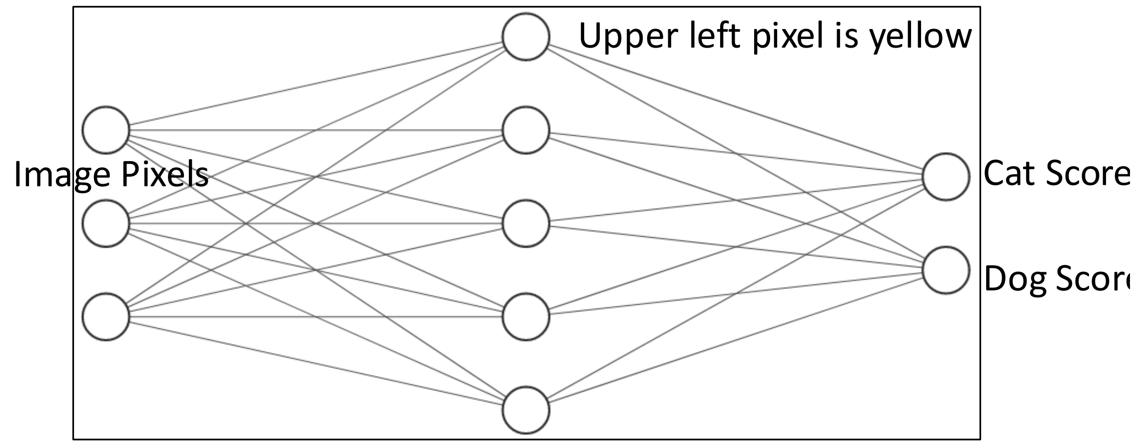
`model.train()` vs `model.eval()`

Remedy: Dropout

We can train the model in such a way that breaks memorization

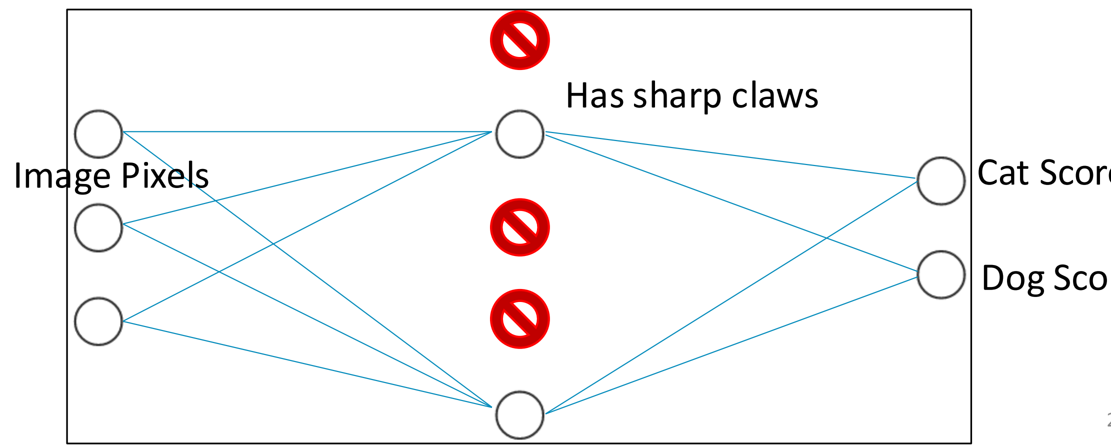
$$Z = A^{[l-1]} W^T + b$$

- Randomly set neuron outputs to zero
- Choose a different set of neurons each time
- The model needs redundant representations
- This leads to more general representations
- A single pathway cannot memorize the input




```
# In model.train() mode
for layer in model.layers():
    keep_prob = 1 - dropout_rate
    keep = torch.rand_like(layer.shape) < keep_prob
    activation *= keep.float()
    activation /= keep_prob

# In model.eval() mode
for layer in model.layers():
    activation *= 1.0
```



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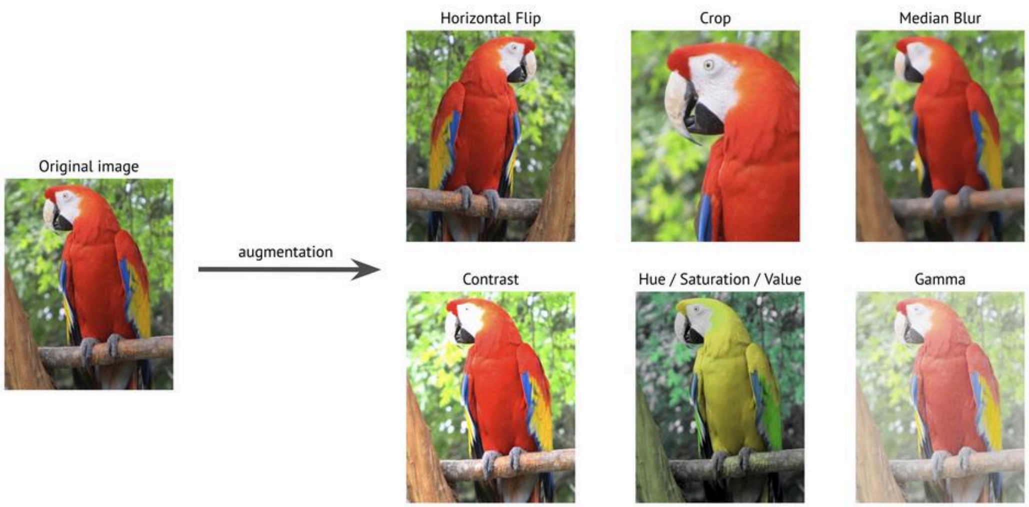
Remedy: Data Augmentation

https://albumentations.ai

Original Mirrored Rotated Brighter

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        loss = criterion(y, yhat)
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    model.eval()
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            metric = metrics(y, yhat, model)
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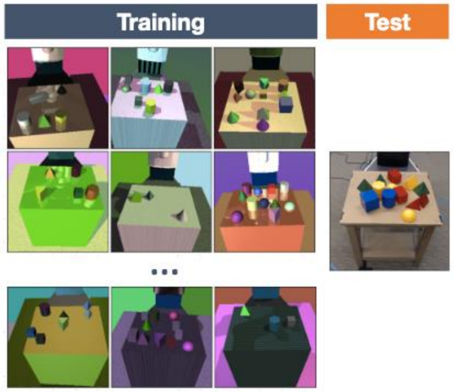
Remedy: Domain Randomization

- This process happens during the data synthesis/creation process.
- It often relies on simulation, and it is frequently used to cross the simulation-to-reality gap.
- This is often called Sim2Real in machine learning and robotics.



"Illustration of our approach. An object detector is trained on hundreds of thousands of low-fidelity rendered images with random camera positions, lighting conditions, object positions, and non-realistic textures. At test time, the same detector is used in the real world with no additional training."

— [Tobin et al]

Summary

- Models can accidentally memorize the input data instead of learning some useful, general property

- We can prevent overfitting/memorization with several remedies

- Most remedies try to
  - Artificially limit the magnitude of parameter values (early stopping, regularization)
  - Add noise and randomness to the training process (dropout, augmentation, domain randomization)

- We often use these remedies together